

Nonadiabatic Quantum Computation by Dynamic Invariants

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We introduce an approach for quantum computing based on the theory of dynamic invariants. This approach generalizes adiabatic quantum computation to a nonadiabatic regime, recovering it as a particular case. We show that the relaxation of adiabaticity can be achieved by processing information in the eigenlevels of a time dependent observable, namely, the dynamic invariant operator. Moreover, we derive the conditions for which the computation can be implemented by time independent as well as by adiabatically varying Hamiltonians. We illustrate our results by providing the implementation of both Deutsch-Jozsa and Grover algorithms via dynamic invariants.

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I. INTRODUCTION

Quantum information processing can be implemented through different quantum computation (QC) models. One promising such a model is provided by adiabatic QC (AQC) [1]. In AQC, rather than using a circuit of unitary quantum gates as in the standard QC model (SQC), an algorithm is implemented via the slow continuous evolution of a time dependent Hamiltonian $H(t)$. The quantum system is prepared in some simple eigenstate $|n(0)\rangle$ of the initial Hamiltonian $H(0)$ and is then allowed to evolve adiabatically so that it remains in the corresponding instantaneous eigenstate $|n(t)\rangle$ of $H(t)$ at all times. At the end of the process, the solution of the problem is encoded in the final state of the system, whence it can be read out by means of a convenient measurement. AQC schemes have been proposed based on superconducting flux qubits [2, 3] and experimentally implemented using nuclear magnetic resonance techniques [4]. Protection of AQC against decoherence has been investigated in several works [5, 6, 7, 8, 9, 10], settling AQC as a favorable approach for QC in real (open) quantum systems.

Inspired by AQC, the aim of this work is to propose a new approach to perform QC via continuous evolution in Hilbert space which is based on the theory of dynamic invariants introduced by Lewis and Riesenfeld [11, 12]. The theory of dynamic invariants was conceived as a tool to solve time dependent problems in quantum mechanics. In turn, as a first application, it was used to discuss the nonadiabatic dynamics of a time dependent harmonic oscillator [11]. Since then, the dynamic invariants technique has been applied to a number of problems which range from quantum optics [13, 14, 15] to atomic systems [16, 17]. More recently, it has also been ap-

plied to the generalization of the concept of geometric phases to nonadiabatic evolutions in open quantum systems [18, 19]. In the present work, we will show that dynamic invariants can be used to implement a nonadiabatic approach to perform QC. In QC by dynamic invariants (QCDI), the computation process will be developed in an arbitrary eigenstate (here chosen as the ground state) of a time dependent quantum observable – the so-called dynamic invariant operator, which will conveniently be defined below. The procedure is somewhat similar to AQC, but it is independent of the adiabatic approximation. Indeed, this is a remarkable feature since the standard form of the adiabatic theorem [20] has recently been subject of controversy, with a number of improvements and new derivations proposed (e.g., see Refs. [21, 22, 23, 24, 25]). Moreover, our method allows for achieving the final (target) state in a nonprobabilistic way. This is in contrast with AQC, where the probability of finding out the solution is directly related with the adiabatic time condition

$$\max_{0 \leq t \leq T} \left| \hbar \frac{\langle n(t) | \frac{dH}{dt} | m(t) \rangle}{(E_n(t) - E_m(t))^2} \right| \ll 1 \quad (m \neq n), \quad (1)$$

where T is the total time of evolution, H is the Hamiltonian of the system, and $\{|n(t)\rangle\}$ and $\{E_n(t)\}$ denote the set of eigenstates and eigenvalues of H , respectively [26]. As a by-product of our approach, we will also show how to recover SQC (via the simulation of constant Hamiltonians) and AQC as particular cases. This is achieved by setting up the conditions for which the Hamiltonian used to implement the quantum algorithm can be chosen to be time independent or adiabatically varying. Hence, QCDI will be proposed as a method which enables us to bring QC to a broader scenery, regaining some other QC models as particular cases. As an illustration, we will provide implementations of QCDI for the Deutsch-Jozsa as well as the Grover algorithms. In particular, the Deutsch-Jozsa algorithm will be studied through the application of different kinds of interpolations between

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the initial and final Hamiltonians, which will reveal the versatility of dynamic invariants for the implementation of QC by continuous evolution.

The paper is organized as follows. In Section II, we review the theory of dynamic invariants. The QCDI method is described in Section III, followed by the analysis of interpolations schemes in Section IV. Section V illustrates QCDI in both the Deutsch-Jozsa and Grover algorithms. In Section VI, conclusions and perspectives are briefly discussed.

II. THEORY OF DYNAMIC INVARIANTS

For a closed system, a dynamic invariant $I(t)$ is defined as an Hermitian operator I which satisfies [11, 12]

$$\frac{\partial I(t)}{\partial t} + \frac{i}{\hbar} [H(t), I(t)] = 0, \quad (2)$$

where H is the Hamiltonian of the system and, from now on, \hbar will be set to one. Dynamic invariants are quantum mechanical constants of motion, implying therefore that their expectation values are constant, i.e., $d\langle I(t) \rangle / dt = 0$. The construction of such an operator allows for the direct integration of the time-dependent Schrödinger equation

$$H(t)|\psi(t)\rangle = i|\dot{\psi}(t)\rangle, \quad (3)$$

with the dot symbol denoting time derivative. Let us consider an instantaneous orthonormal eigenbasis for $I(t)$

$$I(t)|\varphi_i(t)\rangle = \lambda_i|\varphi_i(t)\rangle, \quad (4)$$

where we assume, for simplicity, that the $I(t)$ has non-degenerate eigenlevels. Then, we expand the wave function $|\psi(t)\rangle$ in the invariant operator basis $\{|\varphi_i(t)\rangle\}$, yielding

$$|\psi(t)\rangle = \sum_i c_i(t)|\varphi_i(t)\rangle. \quad (5)$$

By inserting Eq. (5) in Eq. (3) and projecting the result onto $\langle\varphi_j(t)|$ we obtain

$$\dot{c}_j = - \sum_i c_i \langle i|\varphi_j|H|\varphi_i\rangle + \langle\varphi_j|\dot{\psi}\rangle. \quad (6)$$

On the other hand, taking the derivative of Eq. (4) and projecting it onto $\langle\varphi_j(t)|$ we get

$$\dot{\lambda}_i \delta_{ij} + (\lambda_i - \lambda_j) \langle i|\varphi_j|H|\varphi_i\rangle + \langle\varphi_j|\dot{\psi}\rangle = 0.$$

The equation above implies that

$$i = j : \dot{\lambda}_i = 0 \Rightarrow \lambda_i = \text{constant}, \quad (7)$$

$$i \neq j : \langle\varphi_j|\dot{\psi}\rangle = -i\langle\varphi_j|H|\varphi_i\rangle. \quad (8)$$

Eq. (7) is a direct consequence of $I(t)$ being a constant of motion. Concerning Eq. (8), it allows for the integration of Schrödinger equation. Indeed, use of Eq. (8) into Eq. (6) yields

$$c_j(t) = c_j(0) \exp \left[- \int_0^t d\tau \left(\langle\varphi_j|\frac{\partial}{\partial \tau}|\varphi_j\rangle + i\langle\varphi_j|H|\varphi_j\rangle \right) \right].$$

Therefore, if we initially prepare the system in the eigenstate $|\varphi_j(0)\rangle$ of $I(t)$ then the system will necessarily evolve to $|\varphi_j(t)\rangle$ for any time t . The nontransitional evolution of an eigenstate of $I(t)$ plays the role of the adiabatic evolution of an eigenstate of $H(t)$ [20, 26]. As we will show, this suitably built evolution in Hilbert space can be used to perform QC with no adiabatic constraint.

III. QUANTUM COMPUTATION BY DYNAMIC INVARIANTS

Let us now introduce a mechanism to perform QCDI. First, before the definition of the Hamiltonian operator H , we introduce a time dependent dynamic invariant $I(s)$, where s denotes the normalized time, namely, $s = t/T$, with T standing for the total evolution time and $0 \leq s \leq 1$. The operator $I(s)$ is constructed such that: (a) $I(0)$ has a nondegenerate ground state exhibiting a simple structure. (b) $I(1)$ has a nondegenerate ground state which contains the solution of the problem. Similarly to AQC, this can be obtained by providing an eigenvalue penalty for any state that violates the solution to be found. (c) $I(s)$ is defined, for intermediary values of s ($0 < s < 1$), by a conveniently chosen interpolation. As a second step, we can determine the Hamiltonian under which the system will be evolved by imposing that $I(s)$ is a dynamic invariant. This is done here after the definition of $I(s)$ and can be achieved by imposing Eq. (2) which, in terms of the normalized time s , becomes

$$\frac{\partial I(s)}{\partial s} + iT[H(s, T), I(s)] = 0. \quad (9)$$

Finally, we prepare the system in the ground state $|\varphi_0(0)\rangle$ of $I(0)$ and let it evolve during a fixed evolution time T . The system will then be naturally led to the corresponding ground state $|\varphi_0(1)\rangle$ of $I(1)$, since $I(s)$ is built (by definition) as a dynamic invariant. As the solution of the problem is encoded in $|\varphi_0(1)\rangle$, then it can be read out from a suitable measurement. It is worth mentioning that in AQC the probability to obtain the correct final state at the time $s = 1$ goes as the inverse of the gap squared. Therefore, there will be in general a small but nonvanishing probability for AQC to fail. On the other hand in the nonadiabatic approach introduced here (QCDI) the correct final state $|\varphi_0(1)\rangle$ is reached with absolute certainty.

The form of Eq. (9) gives a unitary evolution for $I(s)$, i.e.,

$$I(s) = \tilde{U}(s)I(0)\tilde{U}^\dagger(s), \quad (10)$$

where $\tilde{U}(s)$ is the unitary evolution operator, provided that $H(s, T)$ is Hermitian, and $I(0)$ is the invariant operator at $s = 0$, which one may be written as

$$I(0) = \mathbf{1} - |\varphi_0(0)\rangle\langle\varphi_0(0)|. \quad (11)$$

The unitary interpolation for $I(s)$ given in Eq. (10) has the desirable feature of preserving the spectral gaps

among the eigenvalues of $I(s)$ during all the evolution [27]. This ensures the absence of level crossings in the spectrum of $I(s)$. Note that the ground state of $I(0)$ is $|\varphi_0(0)\rangle$. Then, unless a global phase factor, the final state of the computation $|\varphi_0(1)\rangle$ can be obtained from the initial state $|\varphi_0(0)\rangle$ through a unitary transformation U' : $|\varphi_0(1)\rangle = U'|\varphi_0(0)\rangle$, with $\tilde{U}(1) = U'$. Naturally, U' could in general be written as a sequence of simpler unitary transformations. The corresponding invariant whose ground state is $|\varphi_0(1)\rangle$ is given by

$$I(1) = \mathbf{1} - |\varphi_0(1)\rangle \langle \varphi_0(1)|. \quad (12)$$

Note that no adiabaticity constraint is imposed on the evolution of the invariant operator $I(s)$, and consequently on the state $|\varphi_0(s)\rangle$. If we allow for an adiabatic evolution of $I(s)$, i.e., by using that $\partial I(s)/\partial s \simeq 0$, we obtain from Eq. (9) that the eigenstates of $I(s)$ become also eigenstates of the Hamiltonian, since $[H(s, T), I(s)] \simeq 0$. Hence, we may obtain AQC as a particular case of QCDI, where the necessity of unitary interpolation of the invariant, given by Eq. (10), turns out to be unnecessary.

IV. INTERPOLATIONS OF $I(s)$

In this section we consider different kinds of interpolations of the invariant operator $I(s)$. First we analyze the situation where the Hamiltonian $H(s)$ commute with the evolution operator $\tilde{U}(s)$ for every times s , i.e., time-ordering in the expansion of $\tilde{U}(s)$ is unimportant. In this case, we will show that QC will be implemented by a time independent Hamiltonian. Afterwards we analyze the situation where $H(s)$ does not commute with $\tilde{U}(s)$. In this case, the theory of dynamic invariants may be an important tool in the design of the Hamiltonian which realizes the quantum algorithm.

A. Time-ordering is unimportant: $[H(s), \tilde{U}(s)] = 0$

Let us consider an arbitrary unitary interpolation of the form

$$\tilde{U}(s) = \exp[-i\alpha(s)U], \quad (13)$$

where $\alpha(s)$ is a real function and the operator U is both *Hermitian* ($U = U^\dagger$) and *unitary* ($UU^\dagger = \mathbf{1}$). By combining these two properties of U we have $U^2 = \mathbf{1}$, which enables us to write Eq. (13) as

$$\tilde{U}(s) = \cos[\alpha(s)] \mathbf{1} - i \sin[\alpha(s)] U. \quad (14)$$

Substituting Eqs. (11) and (14) into Eq. (10), we obtain

$$\begin{aligned} I(s) = & \mathbf{1} - \cos^2 \alpha(s) |\varphi_0(0)\rangle \langle \varphi_0(0)| \\ & - \sin^2 \alpha(s) |\varphi_0(1)\rangle \langle \varphi_0(1)| + \frac{i}{2} \sin[2\alpha(s)] \\ & \times [|\varphi_0(1)\rangle \langle \varphi_0(0)| - |\varphi_0(0)\rangle \langle \varphi_0(1)|]. \end{aligned} \quad (15)$$

For $s = 0$ and $s = 1$ Eq. (15) must be reduced to Eqs. (11) and (12), respectively. These requirements lead to the following boundary conditions on $\alpha(s)$:

$$\alpha(0) = n\pi \quad \text{and} \quad \alpha(1) = (n + \frac{1}{2})\pi, \quad \text{with} \quad n \in \mathbb{Z}. \quad (16)$$

Bearing in mind the conditions found in Eq. (16), the final state $|\varphi_0(1)\rangle$ is, unless a global phase factor, given by

$$|\varphi_0(1)\rangle = U|\varphi_0(0)\rangle. \quad (17)$$

Note that Eq. (16) may also be obtained from Eq. (14) by using that $\tilde{U}(0) = \mathbf{1}$ and $\tilde{U}(1)|\varphi_0(0)\rangle = U|\varphi_0(0)\rangle$. To find the Hamiltonian that implements the interpolation given by Eq. (13), we propose

$$H(s, T) = h(s)U. \quad (18)$$

By using Eqs. (15) and (18) into Eq. (9), we get

$$h(s) = \frac{1}{T} \frac{d\alpha(s)}{ds}.$$

Since $\alpha(s) \in \mathbb{R}$, we conclude that $h(s) \in \mathbb{R}$. Then, for the situation in which $U^2 = \mathbf{1}$, the general form of the Hamiltonian $H(s, T)$ that generates the dynamics governed by operator (13) is

$$H(s, T) = \frac{1}{T} \frac{d\alpha(s)}{ds} U. \quad (19)$$

Remarkably, QCDI can be implemented, under certain conditions, via a time independent Hamiltonian. For this purpose, we should choose the function $\alpha(s)$ as

$$\alpha(s) = \frac{\pi s}{2}, \quad (20)$$

with the resulting Hamiltonian reading

$$H(s) = \frac{\pi}{2T} U. \quad (21)$$

Hence we have proved that the unitary interpolation of the dynamic invariant allows for QC with the time independent Hamiltonian (21) as long as U is unitary and Hermitian. By using Eq. (21) and Eq. (13) into Eq. (10), we obtain $I(t) = \exp(-iHt)I(0)\exp(iHt)$, which implies that the unitary evolution of $I(t)$ is implemented by the evolution operator $\exp(-iHt)$ of the system. Note that the total time T appearing in Eq. (21) is inversely related to the gap of H , i.e. a larger gap will contribute to a smaller run time of the algorithm. This is naturally in agreement with AQC. Moreover, the run time in QCDI will be also associated with the ability of simulate efficiently the unitary transformation U , since it can involve nonlocal (many-body) interactions.

B. Time-ordering is important: $[H(s), \tilde{U}(s)] \neq 0$

We consider now a general unitary interpolation for the dynamic invariant which evolves $|\varphi_0(0)\rangle$ to $|\varphi_0(1)\rangle$. This interpolation can be written as

$$\tilde{U}(s) = \exp \left[i \sum_{i=1}^N f_i(s) O_i \right], \quad (22)$$

with $f_i(s)$ being real functions of time and O_i time independent Hermitian operators. Since we are concerned with a general form of the functions $f_i(s)$, it might be a hard task to obtain the Hamiltonian that implements the evolution operator given in Eq. (22). A naive procedure to work out H is to try a direct solution of Schrödinger equation

$$i \frac{\partial \tilde{U}(s)}{\partial s} = T H(s, T) \tilde{U}(s). \quad (23)$$

The application of this procedure is indeed adequate when time ordering of $\tilde{U}(s)$ is unimportant, as shown above. However, for $[H(s, T), \tilde{U}(s)] \neq 0$ for any time $s \in [0, 1]$, the solution of Eq. (22) may get much harder, since the exponential should be broken in parts composed by the operators O_i . An alternative route to solve this problem consists in the application of the theory of dynamic invariants as follows.

Let $C_N = \{O_1, \dots, O_N\}$ be the set of operators composing $\tilde{U}(s)$ in Eq. (22). We assume that C_N is a subset of $C_M = \{O_1, \dots, O_M\}$, with $M \geq N$, where the elements of C_M define an arbitrary Lie algebra

$$[O_i, O_j] = \sum_{k=1}^M C_{ij}^k O_k, \quad (24)$$

where C_{ij}^k ($C_{ij}^k = -C_{ji}^k$) is the structure constant. We write $I(0)$ as

$$I(0) = \sum_{i=1}^M \lambda_i(0) O_i, \quad (25)$$

with $\lambda_i(0)$ being real coefficients. Then, substituting (22) and (25) in (10), we obtain

$$\begin{aligned} I(s) &= \sum_{k=1}^M \left\{ \lambda_k(0) + i \sum_{i=1}^N \sum_{j=1}^M f_i(s) C_{ij}^k \lambda_j(0) + \dots \right\} O_k \\ &= \sum_{k=1}^M \lambda_k(s) O_k, \end{aligned} \quad (26)$$

where we have used Eq. (24) to compute the commutators coming from the expression $\tilde{U}(s) O_k \tilde{U}^\dagger(s)$. As the operators O_k are elements of a Lie algebra, we take the

Hamiltonian of the system as a linear combination of such operators

$$H(s, T) = \sum_{k=1}^M h_k(s, T) O_k, \quad (27)$$

with $h_k(s, T) \in \mathbb{R}$. This expansion of H is rather convenient since it ensures that, after evaluating the invariant operator (26), we may obtain the coefficients $h_k(s, T)$ through Eq. (9). Moreover, note that $h_k(s, T)$ can be determined by the solution of a set of coupled linear equations instead of a set of linear differential equations. Particularly, taking qubits as the building blocks of QC, we can always expand the Hamiltonian in terms of tensor product of Pauli spin matrices (satisfying the $su(2)$ algebra) in the form

$$H(s, T) = \sum_{\{k_i\}} h_{1, \dots, n}^{k_1, \dots, k_n}(s, T) \sigma_1^{k_1} \otimes \sigma_2^{k_2} \otimes \dots \otimes \sigma_n^{k_n},$$

where the lower index enumerate n qubits and the upper index refers to the set $\{\mathbf{1}, \sigma^x, \sigma^y, \sigma^z\}$ of identity and Pauli spin-1/2 matrices. The coefficients $h_i^{k_i}(s, T) \in \mathbb{R}$ since $H(s, T)$ is Hermitian.

V. APPLICATIONS

As applications of QC DI, we will discuss both the Deutsch-Jozsa (DJ) and Grover problems. In particular, we will analyze the DJ algorithm for different interpolations, including the cases where $[H(s), \tilde{U}(s)] = 0$ and $[H(s), \tilde{U}(s)] \neq 0$. These illustrations will make clear that the theory of dynamic invariants may provide a useful tool to determine the Hamiltonian that controls the system dynamics during the computation process.

A. Example 1: the Deutsch-Jozsa problem

Given a binary function $f : \{0, 1\}^n \rightarrow \{0, 1\}$ (n is the number of bits) which is promised to be either constant or balanced, the DJ problem consists in determining which type the function is. Here we construct an implementation by dynamic invariants for the optimized version of the algorithm [28]. Let us begin with the simple case $n = 1$. The input state is $|\varphi_0(0)\rangle = |+\rangle$, where $|\pm\rangle = (|0\rangle \pm |1\rangle)/\sqrt{2}$, with $\{|0\rangle, |1\rangle\}$ being the computational basis for the qubit (eigenstates of the Pauli matrix σ^z). The initial dynamic invariant is chosen such that its ground state is $|\varphi_0(0)\rangle$, i.e., $I(0) = \omega |-\rangle\langle -|$, where ω is a free parameter introduced to set the gap between the eigenstates of $I(0)$. Note that $I(0)$ is introduced in a such a way that a penalty is provided for any state having a contribution of $|-\rangle$. Hence $|\varphi_0(0)\rangle$ is its ground state. The DJ problem can be solved by a single computation of the function f through the unitary transformation $U|x\rangle = (-1)^{f(x)}|x\rangle$ ($x \in \{0, 1\}^n$) [28], so that in

the $\{|x\rangle\}$ (computational) basis U is represented by the diagonal matrix $U = \text{diag}[(-1)^{f(0)}, (-1)^{f(1)}]$. In terms of the Pauli matrices the operator U may be written as $U = \xi_+ \mathbf{1} + \xi_- \sigma^z$, where $\xi_{\pm} = (1/2)[(-1)^{f(0)} \pm (-1)^{f(1)}]$. Our implementation requires a final dynamic invariant $I(1)$ such that its ground state is

$$|\varphi_0(1)\rangle = U|\varphi_0(0)\rangle = \xi_+|+\rangle + \xi_-|-\rangle. \quad (28)$$

This is accomplished by a unitary transformation on $I(0)$, i.e., $I(1) = UI(0)U^\dagger$. Note that this is similar to the nonlinear interpolation for the DJ problem proposed in Ref. [6] in the context of AQC (for linear AQC realizations of the DJ algorithm, see Refs. [29, 30]). However, the nonlinear interpolation is implemented here on $I(s)$ instead of being realized on $H(s)$. The final dynamic invariant encodes the solution of the DJ problem in its ground state, which can be extracted via a measurement of the qubits in the basis $\{|+\rangle, |-\rangle\}$. Indeed, for a constant function, we obtain $\xi_+ = \pm 1$ and $\xi_- = 0$. Then $|\varphi_0(1)\rangle = |+\rangle$ (up to a possible global phase). On the other hand, for a balanced function, we have $\xi_+ = 0$ and $\xi_- = \pm 1$. Then $|\varphi_0(1)\rangle = |-\rangle$ (up to a possible global phase). Following the reasoning developed in the Section IV [see Eqs. (10) and (13)], explicit evaluation of $I(s)$ yields

$$I(s) = \frac{\omega}{2} \{ \mathbf{1} - \cos[2\alpha(s)\xi_-] \sigma^x - \sin[2\alpha(s)\xi_-] \sigma^y \}. \quad (29)$$

Since the operator U displays the properties $UU^\dagger = \mathbf{1}$ and $U = U^\dagger$, we can implement the algorithm through the Hamiltonian

$$H(s, T) = \frac{1}{T} \frac{d\alpha(s)}{ds} U = \frac{1}{T} \frac{d\alpha(s)}{ds} (\xi_+ \mathbf{1} + \xi_- \sigma^z). \quad (30)$$

Hence, by controlling the time variation of $\alpha(s)$ and the frequency T^{-1} we can optimize the run time of the algorithm with no constraint in time.

1. Constant Hamiltonian

As shown in Subsection IV A, it is possible to choose a time-independent Hamiltonian by adjusting $\alpha(s) = \pi s/2$ according to Eq. (20). Then, the Hamiltonian becomes

$$H(s, T) = \frac{\pi}{2T} (\xi_+ \mathbf{1} + \xi_- \sigma^z). \quad (31)$$

Note that H is independent of s , but it goes as the inverse of T . So QCDI for the Deutsch problem can be performed in an arbitrarily short time as long as we are able to ensure an arbitrarily large gap. Observe that H is diagonal. If f is constant, H is simply the identity operator whereas if the function is balanced, H is given by the Pauli matrix σ^z . Note also that the Hamiltonian given in Eq. (31) can be easily simulated by SQC.

2. Oscillating Hamiltonian

When the time derivative of $\alpha(s)$ is not a constant function, we obtain time dependent Hamiltonians. In order to exemplify this situation, we suppose that $\alpha(s)$ has the following form

$$\alpha(s) = \frac{\pi}{2} \sin\left(\frac{\pi s}{2}\right). \quad (32)$$

By using Eq. (19), the Hamiltonian which governs the dynamics reads

$$H(s, T) = \omega(s, T) (\xi_+ \mathbf{1} + \xi_- \sigma^z), \quad (33)$$

where

$$\omega(s, T) = \frac{\pi^2}{4T} \cos\left(\frac{\pi}{2}s\right). \quad (34)$$

Since $\omega(s, T)$ is a time dependent function, we can compute its mean value $\overline{\omega(s, T)}$ in order to obtain the effective frequency associated with $H(s, T)$. Taking an average over the time interval $0 \leq s \leq 1$, we get

$$\overline{\omega(s, T)} = \int_0^1 \omega(s', T) ds' = \frac{\pi}{2T}. \quad (35)$$

Then, by comparing $\overline{\omega(s, T)}$ with the frequency associated with Eq. (31), we observe identical effective frequencies in both examples.

3. Polynomial time dependence of the Hamiltonian

The examples of the Deutsch algorithm explored above belong to the class of interpolations in which the Hamiltonian commute with the evolution operator. In this case, despite its conceptual novelty, the practical usefulness of the theory of dynamic invariants for determining the Hamiltonian might be diminished, since $H(s, T)$ can also be obtained from the evolution operator by directly taking its derivative. Hence, in the situation $[H(s, T), \tilde{U}(s)] = 0$, QCDI can be taken more as a conceptual framework for nonadiabatic QC than as a practical tool to derive new Hamiltonians. However, for $[H(s, T), \tilde{U}(s)] \neq 0$, QCDI provides a systematic approach which is inherently useful for deriving $H(s, T)$. To exemplify this point, let us consider the following form for the evolution operator

$$\tilde{U}(s) = \exp[-i(\nu s^m \sigma_x + \beta s^n \sigma_y + \gamma s^r \sigma_z)], \quad (36)$$

where $\nu, \beta, \gamma \in \mathbb{R}$ and $m, n, r \in \mathbb{N}_+$. In order to obtain the evolved state, we will rewrite $\tilde{U}(s)$ as

$$\begin{aligned} \tilde{U}(s) &= \exp[-i\hat{v}(s) \cdot \vec{\sigma} \phi(s)/2] \\ &= \cos[\phi(s)/2] \mathbf{1} - i\hat{v}(s) \cdot \vec{\sigma} \sin[\phi(s)/2], \end{aligned} \quad (37)$$

with

$$\begin{aligned}\widehat{v}(s) &= \frac{\vec{v}(s)}{|\vec{v}(s)|} = \frac{\nu s^m \hat{i} + \beta s^n \hat{j} + \gamma s^r \hat{k}}{\sqrt{\nu^2 s^{2m} + \beta^2 s^{2n} + \gamma^2 s^{2r}}}, \\ \phi(s) &= 2|\vec{v}(s)| = 2\sqrt{\nu^2 s^{2m} + \beta^2 s^{2n} + \gamma^2 s^{2r}}.\end{aligned}\quad (38)$$

Applying $\widehat{U}(s)$ onto the initial state $|\varphi_0(0)\rangle = |+\rangle$, we find for the final state

$$\begin{aligned}|\varphi_0(s)\rangle &= \frac{\{|\vec{v}(s)| \cos[|\vec{v}(s)|] - i\nu s^m \sin[|\vec{v}(s)|]\}}{|\vec{v}(s)|} |+\rangle \\ &\quad - \frac{(\beta s^n + i\gamma s^r)}{|\vec{v}(s)|} \sin[|\vec{v}(s)|] |-\rangle.\end{aligned}\quad (39)$$

We must be able to obtain the solution of the Deutsch problem from $|\varphi_0(1)\rangle$. One possible way to reach this goal is adjusting $\nu = 0$ and $\beta = \gamma = \pi\xi_+/(2\sqrt{2})$, so that $|\varphi_0(s)\rangle$ becomes

$$\begin{aligned}|\varphi_0(s)\rangle &= \cos\left(\frac{\pi\xi_+}{2}\sqrt{\frac{s^{2n} + s^{2r}}{2}}\right) |+\rangle \\ &\quad - \left(\frac{s^n + is^r}{\sqrt{s^{2n} + s^{2r}}}\right) \sin\left(\frac{\pi\xi_+}{2}\sqrt{\frac{s^{2n} + s^{2r}}{2}}\right) |-\rangle.\end{aligned}\quad (40)$$

Particularly, at time $s = 1$, the state of the system acquires the form

$$|\varphi_0(1)\rangle = \cos\left(\frac{\pi\xi_+}{2}\right) |+\rangle - \left(\frac{1+i}{\sqrt{2}}\right) \sin\left(\frac{\pi\xi_+}{2}\right) |-\rangle.\quad (41)$$

Then, for $s = 1$ we obtain (unless a global phase factor) the state $|\varphi_0(1)\rangle = |+\rangle$ for $f(x)$ balanced ($\xi_+ = 0$) and $|\varphi_0(1)\rangle = |-\rangle$ for $f(x)$ constant ($\xi_+ = \pm 1$). In other words, by measuring the states $|+\rangle$ or $|-\rangle$ we discover whether the function is balanced or constant, respectively.

By taking the coefficients ν , β , and γ as discussed above, the operators $\widehat{U}(s)$ and $I(s)$ become

$$\widehat{U}(s) = \exp\left[-i\frac{\pi\xi_+}{2\sqrt{2}}(s^n\sigma_y + s^r\sigma_z)\right]\quad (42)$$

and

$$\begin{aligned}I(s) &= \frac{1}{2}\left[\mathbf{1} - \cos\left(\pi\xi_+\sqrt{\frac{s^{2n} + s^{2r}}{2}}\right)\sigma_x\right. \\ &\quad + \frac{s^r}{\sqrt{s^{2n} + s^{2r}}}\sin\left(\pi\xi_+\sqrt{\frac{s^{2n} + s^{2r}}{2}}\right)\sigma_y \\ &\quad \left.- \frac{s^n}{\sqrt{s^{2n} + s^{2r}}}\sin\left(\pi\xi_+\sqrt{\frac{s^{2n} + s^{2r}}{2}}\right)\sigma_z\right]\end{aligned}\quad (43)$$

To obtain the Hamiltonian responsible by the evolution of the state (40), we take it as a linear combination of the Pauli matrices, i.e.,

$$H(s, T) = h_x(s, T)\sigma^x + h_y(s, T)\sigma^y + h_z(s, T)\sigma^z,\quad (44)$$

whose coefficients $h_k(s, T)$ ($k = x, y, z$) are determined by the replacement of Eqs. (43) and (44) into (9). Hence, $H(s, T)$ is found to be

$$\begin{aligned}H(s, T) &= -\frac{(ns^{2n-1} + rs^{2r-1})}{2\sqrt{2}T(s^{2n} + s^{2r})}\left[\frac{2\sqrt{2}(n-r)s^{n+r-1}}{(ns^{2n-1} + rs^{2r-1})}\sigma_x\right. \\ &\quad \left.+ \pi\xi_+s^n\sigma_y + \pi\xi_+s^r\sigma_z\right].\end{aligned}\quad (45)$$

Note that the Hamiltonian given by Eq. (45) arises naturally from the theory of dynamic invariants while derivation from Eq. (23) may be clumsy. This simple example illustrates the advantage of dynamical invariants when we are dealing with general evolution operators. In the particular case where $n = r$, the Eq. (45) turns out to be

$$H(s, T) = -\frac{\pi ns^{n-1}}{2\sqrt{2}T}\xi_+(\sigma_y + \sigma_z).\quad (46)$$

The Hamiltonian in Eq. (46) is such that it commutes with $\widehat{U}(s)$. For the effective frequency, we find $\overline{\omega_n}(s, T) = \pi/(2\sqrt{2}T)$, which is of the same order as found before.

4. Introducing more qubits: the Deutsch-Jozsa case

We finish the discussion of the Deutsch problem by showing a simple implementation of QCDI for an arbitrary number n of qubits. Consider the initial state

$$\begin{aligned}|\varphi_0(0)\rangle &= \frac{1}{\sqrt{2}}(|0\rangle_1 + |1\rangle_1) \otimes \dots \otimes \frac{1}{\sqrt{2}}(|0\rangle_n + |1\rangle_n) \\ &= \frac{1}{\sqrt{N}} \sum_{i=0}^{N-1} |i\rangle,\end{aligned}$$

where $N = 2^n$ and the state $|i\rangle$ is written in decimal basis. The invariant operator $I(s)$ can be defined by a unitary interpolation as in Eq. (13), but now with U defined as

$$\begin{aligned}U &= \text{diag}\left[(-1)^{f(0)}, \dots, (-1)^{f(N-1)}\right] \\ &= \sum_{i=0}^{N-1} (-1)^{f(i)} |i\rangle \langle i|.\end{aligned}\quad (47)$$

According to Eq. (11) the invariant at $s = 0$ is

$$I(0) = \mathbf{1} - \frac{1}{N} \sum_{i,j=0}^{N-1} |i\rangle \langle j|.\quad (48)$$

Therefore we obtain

$$I(s) = \mathbf{1} - \frac{1}{N} \sum_{i,j=0}^{N-1} \exp\left[i\pi s \xi_-^{(ij)}\right] |i\rangle \langle j|,\quad (49)$$

with $\xi_-^{(ij)} = (1/2)[(-1)^{f(i)} - (-1)^{f(j)}]$. The ground state of $I(1)$, which will be achieved at the end of the evolution,

is given by

$$|\varphi_0(1)\rangle = U |\varphi_0(0)\rangle = \frac{1}{\sqrt{N}} \sum_{i=0}^{N-1} (-1)^{f(i)} |i\rangle. \quad (50)$$

Then, by measuring the qubits in the basis $\{|+\rangle, |-\rangle\}$, we will get that all the qubits are $|+\rangle$ for a constant function f , otherwise the function is balanced. Concerning the Hamiltonian, we obtain

$$H = \frac{\pi}{2T} U = \frac{\pi}{2T} \sum_{i=0}^{N-1} (-1)^{f(i)} |i\rangle \langle i|. \quad (51)$$

Let us analyze how efficiently we can simulate H as given by Eq. (51). Expanding H in the tensor product of the Pauli basis $\{\mathbf{1}, \sigma^x, \sigma^y, \sigma^z\}$, we can see that H will be given by a sum of diagonal terms, which are given by all the combinations of tensor products of $\mathbf{1}$ and σ^z for each qubit. These terms may involve therefore nonlocal interactions among the qubits. Since these interactions are in a tensor product structure we can efficiently simulate them [31]. However, we must guarantee that the number of terms in H grows only polynomially with the number of qubits. This is ensured due to the fact that, since the function is either constant or balanced, the Hamiltonian will be given either by the identity operator $\mathbf{1}_N$ or by one diagonal operator of the basis given by the tensor products $\mathbf{1}$ and σ^z (e.g. for $n = 2$, H will be given in the balanced case by $\mathbf{1} \otimes \sigma^z$, $\sigma^z \otimes \mathbf{1}$, or $\sigma^z \otimes \sigma^z$). Therefore, the number of terms in H will be fixed for any n , which implies that QCDI can efficiently simulate H .

B. Example 2: The search problem

A simple implementation of QCDI for the search problem [32] can be given as follows. We start by proposing an oracle in a general form given by

$$U_0 = \theta |w\rangle \langle w| + \delta (|w\rangle \langle \varphi_0(0)| + |\varphi_0(0)\rangle \langle w|) + \varepsilon |\varphi_0(0)\rangle \langle \varphi_0(0)|, \quad (52)$$

so that $\theta, \delta, \varepsilon \in \mathbb{R}$ and $|w\rangle$ is the target state. The initial state $|\varphi_0(0)\rangle$ can be decomposed as $|\varphi_0(0)\rangle = \alpha |w\rangle + \beta |y\rangle$, where $\langle w | y \rangle = 0$ and $\alpha^2 + \beta^2 = 1$, with $\alpha = \langle w | \varphi_0(0) \rangle$ and $\beta = \langle y | \varphi_0(0) \rangle$ assumed as real constants. In order to rewrite U_0 in terms of $|w\rangle$ and $|y\rangle$ we define the matrices

$$\begin{aligned} \mathbf{1} &= |w\rangle \langle w| + |y\rangle \langle y|, \quad \sigma_y = -i(|w\rangle \langle y| - |y\rangle \langle w|), \\ \sigma_x &= |w\rangle \langle y| + |y\rangle \langle w|, \quad \sigma_z = |w\rangle \langle w| - |y\rangle \langle y|. \end{aligned} \quad (53)$$

Then we can write $U_0 = r_0 \mathbf{1} + \vec{r} \cdot \vec{\sigma}$, where $r_0 = (\theta + \varepsilon + 2\alpha\delta)/2$, $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ and $\vec{r} = (r_x, 0, r_z)$, with $r_x = \beta(\delta + \varepsilon\alpha)$ and $r_z = [\theta - \varepsilon + 2\alpha(\delta + \varepsilon\alpha)]/2$. Disregarding the term proportional to the identity, we introduce the interpolation operator (13) with $\alpha(s)$ given by (20) and U by

$$U = \frac{\vec{r} \cdot \vec{\sigma}}{|\vec{r}|}. \quad (54)$$

Note that U is unitary and Hermitian. Let us determine now the conditions for which $\tilde{U}(s)$ will yield an interpolation between $|\varphi_0(0)\rangle$ and the solution state $|w\rangle$. Indeed $\tilde{U}(0) = \mathbf{1}$ and therefore $\tilde{U}(0)|\varphi_0(0)\rangle = |\varphi_0(0)\rangle$. For the final time we have

$$\tilde{U}(1)|\varphi_0(0)\rangle = -i \left[\frac{(r_x\beta + r_z\alpha)}{|\vec{r}|} |w\rangle + \frac{(r_x\alpha - r_z\beta)}{|\vec{r}|} |y\rangle \right]. \quad (55)$$

Since we want $\tilde{U}(1)|\varphi_0(0)\rangle = \exp(i\phi)|w\rangle$ (where ϕ is an arbitrary unimportant angle), we impose $r_x\alpha = r_z\beta$. From this condition, we obtain $\theta = \varepsilon$. In terms of the vector \vec{r} , this result implies

$$r_x = \beta(\delta + \varepsilon\alpha), \quad r_z = \alpha(\delta + \varepsilon\alpha) \Rightarrow |\vec{r}| = |\delta + \varepsilon\alpha|. \quad (56)$$

Bearing these results in mind, we are then able to build an oracle which allows for the determination of the element under search at the final time $s = 1$. The dynamic invariant $I(s)$ can be defined by encoding $|\varphi_0(0)\rangle$ as its initial ground state and $|w\rangle$ as its final ground state. Indeed, this can be unitarily achieved by adopting the interpolation given by Eqs. (10) and (11), with U defined in Eq. (54), yielding

$$\begin{aligned} I(s) &= \mathbf{1} - \cos^2\left(\frac{\pi}{2}s\right) |\varphi_0(0)\rangle \langle \varphi_0(0)| - \sin^2\left(\frac{\pi}{2}s\right) |w\rangle \langle w| \\ &\quad + \frac{i}{2} \sin(\pi s) (|w\rangle \langle \varphi_0(0)| - |\varphi_0(0)\rangle \langle w|). \end{aligned} \quad (57)$$

Then, the Hamiltonian operator reads

$$H = \frac{\pi}{2T} U = \frac{\pi}{2T} \frac{\vec{r} \cdot \vec{\sigma}}{|\vec{r}|}. \quad (58)$$

Eq. (56) into Eq. (58) implies

$$H = \mp \frac{\pi}{2T} (\beta\sigma_x + \alpha\sigma_z). \quad (59)$$

In order to have both a dynamic invariant and a Hamiltonian which do not depend on knowing the value of $|w\rangle$, we fix $\alpha = 1/\sqrt{N}$, which implies $\beta = \sqrt{(N-1)/N}$. Then, Eq. (59) becomes

$$H = \mp \frac{\pi}{2T\sqrt{N}} (\sqrt{N-1}\sigma_x + \sigma_z). \quad (60)$$

The equation above resembles the Hamiltonian used in Ref. [33] to implement the analog analogue of QC. Simulation of such a kind of Hamiltonian can be implemented by a quantum circuit whose number of oracle calls grows as $O(\sqrt{N})$ [31].

VI. CONCLUSION

In conclusion, we have proposed an approach for continuously implementing QC in Hilbert space which generalizes AQC to a nonadiabatic regime. Our method opens

up the possibility of realizing QC with new (in certain cases fixed) Hamiltonians and with no adiabaticity constraint. Moreover it recovers SQC and AQC as particular cases, running in a nonprobabilistic way. For Hamiltonians which do not commute with the evolution operator, QCDI was shown to provide a systematic tool to obtain the dynamics of the quantum system. Since QC is still in its early stage, the existence of a diversity of QC models can be a valuable way of providing new experimental routes as well as insights for the design of quantum al-

gorithms. Robustness of QCDI under decoherence is an important further point. In this context, a possible direction can be provided by the recent generalization of the theory of dynamic invariants for open systems evolving under convolutionless master equations proposed in Ref. [18]. We leave this analysis for future research.

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